Finite Temperature Many-Body Theory with the Lipkin Model

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Abstract

We have compared exact numerical results for the Lipkin model at finite temperature with Hartree-Fock theory and with the results of including in addition the ring diagrams. In the simplest version of the Lipkin model the Hartree-Fock approach shows a "phase transition" which is absent in the exact results. For more realistic cases, Hartree-Fock provides a very good approximation and a modest improvement is obtained by adding the ring diagrams.

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1 Introduction

The study of hot nuclei and hot nuclear matter is of importance in heavy ion collisions and in supernova explosions. Theoretical treatments require the use of finite-temperature many-body theory which is inherently more difficult than the corresponding zero-temperature formalism. Since in practical situations the many-body theory cannot be solved exactly, approximations are needed and it is often difficult to know how accurate these might be. It is therefore useful to study a model which has some realistic features, but which is sufficiently simple to permit an exact solution, so that the accuracy of various approximations can be assessed. With this objective in mind we shall study here the Lipkin model [1] which has been widely used at zero temperature. Rather little work has been carried out at finite temperature with the Lipkin model [2, 3, 4] and then only for the simplest version of the model. The principle interest in these studies was excited states and boson expansions. Particularly striking was the demonstration that a phase transition can occur in the Hartree-Fock (HF) solutions. We shall point out that the exact internal energy shows a qualitatively different behavior.

In addition to HF we will consider the correlations of the particle-particle hole-hole ring diagrams, *i.e.*, the random phase approximation (RPA), for which an expression for the grand potential has recently been given [5, 6]. We choose these approximations since Yang, Heyer and Kuo [7] found that at zero temperature HF gave a very good approximation to the exact ground state energy and the ring series gave a further small improvement. The final result was therefore very close to the true energy of the system. The

present study can be regarded as the continuation of the work of ref. [7] to finite temperature. An additional motivation for studying the long range correlations of the ring series is that in calculations with realistic interactions it significantly improves the location of the saturation point in nuclear matter [8]. We note in passing that we shall not consider the particle-hole ring series since it gave a negligible effect in the zero temperature work of ref. [7].

The organization of this paper is as follows. In subsec. 2.1 we discuss our method of obtaining exact numerical solutions for a slightly modified version of the original Glick, Lipkin and Meshkov model [1]. The approximate many-body methods with which we compare, namely HF and RPA, are discussed in subsec. 2.2. The comparison of our approximate and exact results is given in sec. 3 and brief concluding remarks are presented in sec. 4.

2 Theory

2.1 Exact Lipkin-Model Calculation

The Lipkin model [1] consists of two single-particle levels labelled by $\sigma = -$ and $+$, each of which has a degeneracy p. We write the Hamiltonian

$$H = H_0 + \mathcal{V} , \quad \text{where}$$

$$H_0 = \tfrac{1}{2}\xi \sum_{p\sigma} \sigma a_{p\sigma}^\dagger a_{p\sigma} , \quad \text{and}$$

$$\mathcal{V} = \tfrac{1}{2}V \sum_{pp'\sigma} a_{p\sigma}^\dagger a_{p'\sigma}^\dagger a_{p'-\sigma} a_{p-\sigma} + \tfrac{1}{2}W \sum_{pp'\sigma} a_{p\sigma}^\dagger a_{p'-\sigma}^\dagger a_{p'\sigma} a_{p-\sigma}$$

$$+ \tfrac{1}{2}U \sum_{pp'\sigma} \left[a_{p\sigma}^\dagger a_{p'\sigma}^\dagger a_{p'-\sigma} a_{p\sigma} + a_{p\sigma}^\dagger a_{p'-\sigma}^\dagger a_{p'\sigma} a_{p\sigma} \right] . \tag{1}$$

Here H_0 is the unperturbed Hamiltonian with single particle energies $\pm\frac{1}{2}\xi$. The two-body interaction, $\mathcal{V}$, has three terms. The interaction V acts between a pair of particles with parallel spins and changes the spins from $++$ to $--$, or *vice versa*. The interaction W is a spin-exchange interaction and U, which was not present in the original model [1], flips the spin of one particle. It is of interest to note that the interaction does not change the value of the degeneracy labels pp'.

Since each particle has only two possible states, the use of the quasi-spin formulation was suggested by Lipkin *et al.* [1]. The quasi-spin operators obey angular momentum commutation relations and are defined by

$$J_z = \tfrac{1}{2}\sum_{p\sigma} \sigma a^\dagger_{p\sigma} a_{p\sigma} \ , \ \ J_+ = \sum_p a^\dagger_{p+} a_{p-} \ , \ \ J_- = \sum_p a^\dagger_{p-} a_{p+} \ . \tag{2}$$

The Hamiltonian can then be compactly expressed in the form

$$H = \xi J_z + \tfrac{1}{2}V(J_+^2 + J_-^2) + \tfrac{1}{2}W(J_+ J_- + J_- J_+ - n) + \tfrac{1}{2}U(J_+ + J_-)(n-1) \ , \tag{3}$$

where the number operator $n = \sum_{p\sigma} a^\dagger_{p\sigma} a_{p\sigma}$. The operator $J^2 = \frac{1}{2}(J_+ J_- + J_- J_+) + J_z^2$ commutes with the Hamiltonian so the Hamiltonian matrix breaks up into submatrices of dimension $2J+1$, each associated with different values of J; for a given number of particles N the largest angular momentum corresponds to $J = \frac{1}{2}N$. It is straightforward to use standard angular momentum techniques to set up these submatrices which can then be diagonalized. Using a label α to distinguish the eigenvalues e, we have $e = e(N, J, \alpha)$.

Having obtained the exact eigenvalues for all N, we can calculate the grand potential corresponding to the grand canonical ensemble according to

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$$\Omega = -\beta^{-1} \ln Z \; , \qquad \text{where}$$

$$Z = \sum_{NJ\alpha} d(N, J) e^{-\beta\{e(N,J,\alpha) - \mu N\}} \; . \tag{4}$$

Here μ is the chemical potential and $\beta = T^{-1}$ is the inverse temperature. The quantity $d(N, J)$ gives the degeneracy, $i.e.$, the number of times the angular momentum J occurs for a given N-particle system. The physical quantities of interest, namely the mean number of particles $\langle N \rangle$ and the internal energy E, can then be obtained from the grand potential with the usual thermodynamic relations

$$\langle N \rangle = -\frac{\partial \Omega}{\partial \mu} \quad , \quad E = \frac{\partial}{\partial \beta}(\beta\Omega) + \mu\langle N \rangle \; . \tag{5}$$

This yields

$$\langle N \rangle = Z^{-1} \sum_{NJ\alpha} N d(N, J) e^{-\beta\{e(N,J,\alpha) - \mu N\}}$$

$$E = Z^{-1} \sum_{NJ\alpha} e(N, J, \alpha) d(N, J) e^{-\beta\{e(N,J,\alpha) - \mu N\}} \; . \tag{6}$$

2.2 Many-Body Approximations

Our basic many-body approach is the Hartree-Fock approximation for which the finite temperature formalism is well known [9]. The HF single particle equations are

$$\epsilon_i \delta_{ik} = \langle k|H_0|i\rangle + \sum_j \langle kj|\mathcal{V}|ij\rangle f_j \; , \tag{7}$$

where HF eigenvectors are used, *i.e.*, $|i\rangle = c_i(+)|+\rangle + c_i(-)|-\rangle$. Also the Fermi occupation probabilities are $f_j = [1 + \exp(\beta\tilde{\epsilon}_j)]^{-1}$ with the definition $\tilde{\epsilon}_j = \epsilon_j - \mu$. The grand potential is then

$$\Omega_{\mathrm{HF}} = -\beta^{-1}\sum_i \ln\left(1 + e^{-\beta\tilde{\epsilon}_i}\right) - \sum_{i>j}\langle ij|\mathcal{V}|ij\rangle f_i f_j \;, \tag{8}$$

from which, using eq. (5), the standard relations follow

$$\langle N\rangle_{\mathrm{HF}} = \sum_i f_i$$

$$E_{\mathrm{HF}} = \sum_i \epsilon_i f_i - \sum_{i>j}\langle ij|\mathcal{V}|ij\rangle f_i f_j \;. \tag{9}$$

Now we also want the grand potential giving the sum of the particle-particle hole-hole ring diagrams. This was evaluated in refs. [5, 6], but actually a much simpler derivation can be given in just a few lines. It is worthwhile to present this here. The ring series takes the form [5, 10]

$$\Omega_{\mathrm{ring}} = \beta^{-1}\sum_\nu e^{i\omega_\nu 0^+}\mathrm{Tr}[F\mathcal{V} - \tfrac{1}{2}(F\mathcal{V})^2 + \tfrac{1}{3}(F\mathcal{V})^3 - \ldots]$$

$$= \beta^{-1}\sum_\nu e^{i\omega_\nu 0^+}\mathrm{Tr}\ln(1 + F\mathcal{V}) \;, \tag{10}$$

where the notation $F\mathcal{V}$ means $F_{ij}(i\omega_\nu)\langle ij|\mathcal{V}|kl\rangle$ and the summation is over $i > j$, *etc.* Here the Matsubara frequency $\omega_\nu = 2\pi\nu T$, with ν running over all integers. It should also be understood that a HF basis is used to evaluate the various quantities which arise. The pair propagator

$$F_{ij}(i\omega_\nu) = -\frac{Q(ij)}{i\omega_\nu - \tilde{\epsilon}_{ij}} \;, \tag{11}$$

where we have introduced the simplifying notation $Q(ij) = (1 - f_i)(1 - f_j) - f_i f_j = 1 - f_i - f_j$ and $\tilde{\epsilon}_{ij} = \tilde{\epsilon}_i + \tilde{\epsilon}_j$. Using a matrix notation, eq. (10) can be written

$$\Omega_{\mathrm{ring}} = \beta^{-1}\sum_\nu e^{i\omega_\nu 0^+}\mathrm{Tr}\ln\left[\frac{(i\omega_\nu - \tilde{\epsilon})\mathbf{1} - Q\mathcal{V}}{(i\omega_\nu - \tilde{\epsilon})\mathbf{1}}\right] \;. \tag{12}$$

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The sum over ν can be performed using eq. (13) of ref. [5] with the result

$$\Omega_{\text{ring}} = \beta^{-1} \text{Tr} \ln \left[\frac{e^{-\beta(\tilde{\epsilon}\mathbf{1} + Q\mathcal{V})} - 1}{e^{-\beta\tilde{\epsilon}\mathbf{1}} - 1} \right] . \tag{13}$$

Choosing a diagonal representation, *viz.*

$$\sum_{k>l} \{ \tilde{\epsilon}_{ij} \delta_{ij,kl} + Q(ij)\langle ij|\mathcal{V}|kl\rangle \} \langle kl|X_n\rangle = \Delta_n \langle ij|X_n\rangle , \tag{14}$$

and noting that Tr ln = ln det, we obtain the final form

$$\Omega_{\text{ring}} = \beta^{-1} \ln \frac{\prod_n (1 - e^{-\beta\Delta_n})}{\prod_{i>j}(1 - e^{-\beta\tilde{\epsilon}_{ij}})} . \tag{15}$$

Thus the grand potential is the difference between that obtained with random phase approximation (RPA) bosons and that obtained with unperturbed fermion pairs, treated as bosons. Now we should not simply add the ring and the HF results because the first order term of eq. (10) has already been included in the HF contribution. Thus we must subtract this, taking

$$\Omega'_{\text{ring}} = \Omega_{\text{ring}} - \sum_{i>j} \langle ij|\mathcal{V}|ij\rangle f_i f_j . \tag{16}$$

Then $\Omega_{\text{total}} = \Omega_{\text{HF}} + \Omega'_{\text{ring}}$.

A simple, but approximate, method of obtaining the thermodynamic quantities of interest is to use the HF result (9) for the average number of particles and take the total energy to be $E_{\text{total}} = E_{\text{HF}} + \Omega'_{\text{ring}}$. This ignores the effect of the derivatives of eq. (5) upon Ω'_{ring} and is therefore easy to compute. We shall comment upon this approximation later. Our aim, however, is to evaluate $\langle N \rangle_{\text{total}}$ and E_{total} exactly within the HF RPA formalism and this requires the derivatives of the HF and RPA energies and the derivative of the HF wavefunctions.

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2.2.1 Evaluation of Derivatives

Consider a general eigenvalue equation for a matrix which may, in general, be non-symmetric

$$\langle \tilde{j}|H|i\rangle = E_i \delta_{ij} \quad \text{with} \quad \langle \tilde{j}|i\rangle = \delta_{ij} \ , \tag{17}$$

where the vectors $|\tilde{i}\rangle$ are the biorthogonal complements to the vectors $|i\rangle$. Denoting partial derivatives with respect to some thermodynamic variable, x, by a prime, we have

$$\langle \tilde{j}'|H|i\rangle + \langle \tilde{j}|H'|i\rangle + \langle \tilde{j}|H|i'\rangle = E_i' \delta_{ij} \ , \tag{18}$$

$$\langle \tilde{j}'|i\rangle + \langle \tilde{j}|i'\rangle = 0 \ . \tag{19}$$

In the diagonal case, $j = i$, these equations give

$$\langle \tilde{i}|H'|i\rangle = E_i' \ , \tag{20}$$

and in the off-diagonal case, $j \neq i$,

$$\langle \tilde{j}|H'|i\rangle = (E_i - E_j)\langle \tilde{j}|i'\rangle \ . \tag{21}$$

For the HF case we are dealing with a symmetric matrix so that $|\tilde{i}\rangle = |i\rangle$. Then applying the above to eq. (7), we have

$$\epsilon_i' \delta_{ik} = (\epsilon_k - \epsilon_i)\langle k|i'\rangle + \sum_j \left[\langle kj'|\mathcal{V}|ij\rangle f_j + \langle kj|\mathcal{V}|ij'\rangle f_j + \langle kj|\mathcal{V}|ij\rangle f_j' \right] . \tag{22}$$

The derivative $f_j' \equiv \frac{\partial f_j}{\partial x} = -f_j(1 - f_j)\frac{\partial}{\partial x}[\beta(\epsilon_j - \mu)]$, which involves the unknown ϵ_j'. The derivatives of the HF wavefunctions are constrained by eq. (19) which implies $\langle i|i'\rangle = 0$ and $\langle j|i'\rangle = -\langle j'|i\rangle$. In our case there are only two states $|i\rangle$, and labelling these $|1\rangle$ and $|2\rangle$, we have

$$|1'\rangle = d|2\rangle \qquad , \qquad |2'\rangle = -d|1\rangle \ , \tag{23}$$

where d is a constant. Thus we have three unknowns ϵ'_1, ϵ'_2 and d and these can be obtained by solving the three independant equations (22). It is also useful to note that eq. (22) yields the relation

$$f_i\epsilon'_i \equiv f_i\frac{\partial\epsilon_i}{\partial x} = \frac{\partial}{\partial x}\left[\sum_{i>j}\langle ij|\mathcal{V}|ij\rangle f_if_j\right] . \tag{24}$$

We also need the derivatives of the RPA eigenvalues Δ_n. Using the vectors $\tilde{X}$ which are biorthogonal to the vectors X, namely

$$\sum_{i>j}\langle\tilde{X}_m|ij\rangle\langle ij|X_n\rangle = \delta_{mn} , \tag{25}$$

it follows from eqs. (14) and (20) that we can write

$$\frac{\partial\Delta_n}{\partial x} = \sum_{i>j,k>l}\langle\tilde{X}_n|ij\rangle\left(\frac{\partial}{\partial x}\left[\tilde{\epsilon}_{ij}\delta_{ij,kl} + Q(ij)\langle ij|\mathcal{V}|kl\rangle\right]\right)\langle kl|X_n\rangle . \tag{26}$$

The derivative of the quantity in square brackets involves ϵ'_i, f'_i and $|i'\rangle$ which, as we have discussed, are obtained from eq. (22).

Using eq. (5) and the grand potential Ω_{total}, we then have the exact expression for the number of particles

$$\langle N\rangle_{\text{total}} = \sum_i f_i\left(1 + \frac{\partial\epsilon_i}{\partial\mu}\right) - \sum_n\left[e^{\beta\Delta_n} - 1\right]^{-1}\frac{\partial\Delta_n}{\partial\mu}$$
$$+ \sum_{i>j}\left[e^{\beta\tilde{\epsilon}_{ij}} - 1\right]^{-1}\frac{\partial\tilde{\epsilon}_{ij}}{\partial\mu} . \tag{27}$$

The internal energy is given by

$$E_{\text{total}} = \sum_i f_i\left(\epsilon_i - \beta\frac{\partial\epsilon_i}{\partial\rho}\right) + \sum_n\left[e^{\beta\Delta_n} - 1\right]^{-1}\left(\Delta_n + \beta\frac{\partial\Delta_n}{\partial\rho}\right)$$
$$- \sum_{i>j}\left[e^{\beta\tilde{\epsilon}_{ij}} - 1\right]^{-1}\left(\tilde{\epsilon}_{ij} + \beta\frac{\partial\tilde{\epsilon}_{ij}}{\partial\rho}\right) - 2\sum_{i>j}\langle ij|\mathcal{V}|ij\rangle f_if_j , \tag{28}$$

where $\frac{\partial}{\partial\rho} \equiv \frac{\partial}{\partial\beta} - \frac{\mu}{\beta}\frac{\partial}{\partial\mu}$.

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3 Calculation and Results

The first step in carrying out the calculations is to compute the two HF energies via eq. (7) which requires that both the wave function amplitudes $c_i(\pm)$ and the occupation probabilities f_i be self-consistent. The derivatives of the HF eigenvalues and eigenfunctions can then be obtained from eq. (22) and the RPA eigenvalue equation (14) solved. Now the chemical potential μ must be chosen to reproduce the correct number of particles. Initially this is done in the HF loop using eq. (9), but once Ω'_{ring} has been computed the number of particles must be obtained from eq. (27). This will no longer be the desired value, so μ has to be adjusted and another iteration carried out and so on until the correct number of particles is obtained.

For the RPA equation (14) we need to consider a five-dimensional basis, since the results are independant of the degeneracy labels p, p'. Specifically the basis is

$$a^\dagger_{p'1}a^\dagger_{p1} \ , \ a^\dagger_{p'1}a^\dagger_{p2} \ , \ a^\dagger_{p'2}a^\dagger_{p1} \ , \ a^\dagger_{p'2}a^\dagger_{p2} \ , \quad p \neq p'$$

$$a^\dagger_{p2}a^\dagger_{p1} \tag{29}$$

where 1 and 2 label the HF states. The RPA matrix actually breaks into a 4×4 matrix (for $p \neq p'$) and a 1×1 matrix ($p = p'$). Although we did not use it to simplify the calculations, we point out that in actuality the 4×4 matrix can be split into a 1×1 matrix corresponding to the linear combination $\left(a^\dagger_{p'2}a^\dagger_{p1} - a^\dagger_{p'1}a^\dagger_{p2}\right)$ and a 3×3 matrix for the orthogonal states.

We shall discuss the case where the available states are half-filled, *i.e.*, $\langle N \rangle = p$, since other choices do not yield qualitatively different results. Also

for the pure HF case the levels 1 and 2 must either be completely filled or completely empty at $T = 0$, so the choice $\langle N \rangle = p$ yields a well-defined $T = 0$ limit. For the half-filled case the pure HF result from eq. (9) requires a chemical potential $\mu = \frac{1}{2}(\epsilon_1 + \epsilon_2)$, which implies that $f_1 + f_2 = 1$ or $Q(12) = Q(21) = 0$. This means that only the $a^\dagger_{p'1} a^\dagger_{p1}$ and $a^\dagger_{p'2} a^\dagger_{p2}$ states yield a non-zero RPA contribution. When the chemical potential is obtained from eq. (27) which employs Ω_{total}, this is no longer precisely true, neverthelesss the contribution of the three "12" states remains small.

We shall present results for the case where $p = 16$ and $\langle N \rangle = 16$ so that half of the 32 available states are filled. We have examined other values of $\langle N \rangle = p$ and found no qualitative differences, although the approximations are quantitatively a little less accurate for smaller numbers of particles, as one might expect. We will take $\xi = 1$, thus implicitly measuring energies in units of ξ, *i.e.*, the quantities we discuss are dimensionless. Further we will choose $U = W$ since no qualitative difference is observed if they are unequal.

For our first set of calculations we chose for the parameters of the Hamiltonian of eq. (1) $U = W = 0$ and $V = -0.65$ so that we can discuss the situation addressed in refs. [2, 3, 4]. With only V non-zero analytical solutions can be obtained for the pure HF case [3, 4]. Defining $\epsilon_1 = -\epsilon_2 = -\frac{1}{2}\epsilon^{\text{HF}}$, a solution with $\epsilon^{\text{HF}} = 1$ is always possible, *i.e.*, in this case the HF Hamiltonian is unchanged from the unperturbed Hamiltonian, H_0. However, if it exists, the solution of

$$\epsilon^{\text{HF}} = |V|(p - 1) \tanh \tfrac{1}{4}\beta\epsilon^{\text{HF}} \tag{30}$$

gives a lower energy [3, 4]. As T increases, *i.e.*, β decreases, the tanh de-

creases until the limiting case is reached where $\epsilon^{\mathrm{HF}} = 1$; for our parameter choice the critical temperature $T_c = 2.43$. This behavior is illustrated by the dashed curve in fig. 1 where we plot the lower eigenvalue ϵ_1. The numbers on the curves indicate the intensity $c_1(-)^2$. This starts out at 0.55 and becomes unity after the phase transition to the unperturbed state. The corresponding internal energy, E_{HF}, is shown as a function of temperature in fig. 2 (dashed curve). At the phase transition the slope becomes discontinuous and for higher temperatures the energy arises from the unperturbed Hamiltonian, H_0, only. This can be contrasted with the exact result denoted by diamonds in fig. 2 where the curve is smooth and there is no indication of a phase transition. We conclude that the discontinuity is an artifact of the approximation which is employed, without physical significance. The effect of including the ring diagrams is indicated by the solid curve in fig. 2. We see that that they yield a modest improvement in the results at low temperatures, in agreement with the zero-temperature results of ref. [7]. At fairly high temperatures the effect is larger and brings the calculations close to the exact result. However, the rings yield a discontinuous curve in the "phase transition" region and the results are inaccurate there. We remark in passing that a similar "phase transition" appears for the case $U = V = 0$ with $W \neq 0$ and again the exact calculations show no evidence for such an effect.

We may note that, as $T \to \infty$, the occupation probabilities $f_i \to \frac{1}{2}$ and therefore $Q(ij) \to 0$ so that the RPA energies Δ_n of eq. (14) are just the HF energies $\tilde{\epsilon}_{ij}$. It is straightforward to check that in this limit $\Omega'_{\mathrm{ring}} \to 0$. The

internal energy is just the HF energy which can be written

$$E_\text{total} = E_\text{HF} = \tfrac{1}{4}\sum_{i>j}\langle ij|\mathcal{V}|ij\rangle = -\tfrac{1}{4}pW \ . \tag{31}$$

Since the pair propagator vanishes $(Q(ij) \to 0)$ and the particle-hole propagator also vanishes (because it is proportional to $[(1 - f_i)f_j - f_i(1 - f_j)]$ which is zero in this limit) this should be an exact result. That is, at infinite temperature only contributions of first order in $\mathcal{V}$ survive. We have verified that eq. (31) agrees with the results of our exact calculations. For the case shown in fig. 2, eq. (31) implies that the asymptotic internal energy is zero.

We next examine the effect of taking the relatively modest values $U = W = -0.02$, with the same value of $V = -0.65$. The results for this case are given in fig. 3. As compared with fig. 2, the change in the internal energy is small and the exact results are quite similar in the two cases. However there is a qualitative difference for the HF curve which now smoothly approaches the unperturbed result for high temperatures. The unperturbed case, which arises from H_0 and is the same for all the calculations we present, is represented by the dot-dashed curve in fig. 3. Comparing this to the other curves at low temperatures, we see that the effect of the perturbation $\mathcal{V}$ is very large indeed . The corresponding HF single particle energy and intensity in fig. 1 are similar to before except, that there is no phase transition and that asymptotically for $T \to \infty$ the intensity $c_1(-)^2 \to 0.98$ rather than unity. The effect of including the ring diagrams here is shown by the solid curve of fig. 3. This differs from the previous case in the region where the transition from the low to the high temperature behavior takes place– the curve is now smooth and the agreement with the exact results is much better.

As a final case we take $U = W = -0.2$, these values being comparable to V, which again is -0.65. The results in fig. 4 show that the internal energy, E, is roughly doubled at low temperature and the pure HF approximation gives very good agreement with the exact answer. The effect of the ring digrams is small, but they do provide even better results at high temperatures. Reducing the rather large value of V that we have used to make it comparable to or less than U and W results in even less of an effect from the ring diagrams. This is not unexpected since the matrix element between the 11 and 22 states dominates the RPA correlations and this is strongly influenced by V. The single particle energies here (solid curve of fig. 1) are much larger than in the previous examples and the mixing between the basis states remains large at high temperature. In fact for $T \to \infty$ the intensity $c_1(-)^2 \to 0.66$.

Finally let us discuss the approximation of taking $E = E_{\mathrm{HF}} + \Omega'_{\mathrm{ring}}$. As $T \to 0$ the quantity $f_j(1 - f_j)$ goes exponentially to zero, in which case eq. (22) indicates that the derivatives of the HF energies and wavefunctions become zero. Thus setting the derivative contributions in eq. (28) to zero, the $T = 0$ ring contribution to the energy is just $-(\sum_n \Delta_n - \sum_{i>j} \tilde{\epsilon}_{ij})$, where the summation runs over those states for which Δ_n and $\tilde{\epsilon}_{ij} < 0$. In other words the states with energies less (greater) than the chemical potential are filled (unfilled). The same expression is obtained directly from Ω_{ring} in eq. (15) and this is the well-known $T = 0$ result [5, 6]. Thus, at $T = 0$, the internal energy is exactly given by $E_{\mathrm{HF}} + \Omega'_{\mathrm{ring}}$. However as the temperature increases this becomes an approximation and it begins to deteriorate when the slope of the internal energy curves in figs. 2–4 starts to increase. Indeed

Ω'_{ring} is always negative, whereas $(E_{\text{total}} - E_{\text{HF}})$ is positive in some regions. In the high temperature regime $E_{\text{HF}} + \Omega'_{\text{ring}}$ gives energies that are roughly halfway between the HF and the HF+ring results. Thus the accuracy of this approximation can only be relied upon at low temperatures.

4 Concluding Remarks

We have calculated the thermodynamic properties of the Lipkin model Hamiltonian exactly and compared with approximate many-body treatments. The case where only the V (or only the W) term of the Hamiltonian is non-zero is special because the Hartree-Fock single particle states differ from the unperturbed values only for temperatures up to some critical T_c. The transition between the two situations manifests itself as a discontinuity in the slope of the calculated quantities. However no such effect is observed in the exact calculations. Further if the other parameters of the Hamiltonian are allowed to differ from zero, even by a relatively small amount, this behavior of the HF theory disappears and the calculated curves are smooth with no discontinuities in the derivatives. For both of these reasons we conclude that the HF "phase transition" is an artifact which is not likely to be relevant to actual physics.

In cases where all the parameters of the Hamiltonian are non-zero, which we think is much more likely to be representative of actual situations, we find very good agreement between the exact and the HF results. We found this somewhat surprising since the differences between the exact and the unperturbed internal energies can be large, *i.e.*, the perturbation is not in any

sense small. We also examined the effects of the particle-particle ring series and found that accuracy demands a thermodynamically correct treatment of this contribution, *i.e.*, the number of particles and the internal energy should be obtained from the thermodynamic relations (5) using the complete grand potential Ω_{total}. The ring effects yield a modest improvement of the HF result which is mainly evident at high temperatures, although there is a small effect in the low-T regime. Regarding the ring contribution, we make two cautionary remarks. Firstly we have used a rather large value of the parameter V so as to investigate the situation discussed in the previous paragraph; this has the effect of enhancing the size of the rings. Secondly in the infinite temperature limit we have pointed out that the ring contribution becomes zero. Nevertheless our full approximation is remarkably accurate and it would be interesting to see what results it yields for more realistic Hamiltonians.

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Figure Captions

Figure 1. The Hartree-Fock energy of the lower state, ϵ_1, as a function of temperature for the three different parameter sets indicated. The numbers indicate the intensity of the $|-\rangle$ component of the corresponding eigenvector, i.e., $c_1(-)^2$.

Figure 2. Comparison of the HF, the HF and ring diagram and the exact values of the internal energy as a function of temperature. The three cases are denoted respectively by the dashed curve, solid curve and by diamonds. The parameters are $V = -0.65$, $U = W = 0$.

Figure 3. As for fig. 2, but with parameters $V = -0.65$, $U = W = -0.02$. Here the dot-dashed curve gives the result obtained with the unperturbed Hamiltonian, H_0, only.

Figure 4. As for fig. 2, but with parameters $V = -0.65$, $U = W = -0.2$.